

## **Appendix B**

### **Properties of Common Organic Pollutants**

#### **B-1. Introduction**

Appendix B consists of 13 tables, each presenting physical and/or chemical properties of compounds and fuel products. This information, including, for example, molecular weights, boiling points, Henry's Law Constants, vapor pressures, and vapor densities may prove helpful in evaluating whether a given site with its contaminants of concern is amenable to SVE/BV. In addition, this information may be needed in calculating various operating parameters or outcomes of an SVE/BV system at a given site with a given suite of contaminants of concern.

#### **B-2. List of Tables**

- B-1: Selected Compounds and Their Chemical Properties. Lists molecular weight, compound boiling point, vapor pressure, and equilibrium vapor concentration.
- B-2: Physicochemical Properties of PCE and Associated Compounds. Lists molecular weight, liquid density, melting point, boiling point, vapor pressure, water solubility, log octanol-water coefficient, soil sorption coefficient, and Henry's Law constant for PCE; TCE; 1,1-DCE; 1,2-DCE; and vinyl chloride.
- B-3: Physicochemical Properties of TCA and Associated Compounds. Lists same properties as Table B-2 for 1,1,1-TCA; 1,1-DCA; and CA.
- B-4: Physical Properties of Fuel Components. Lists molecular weight, solubility, soil sorption coefficient, log octanol-water coefficient, and vapor pressure for n-alkanes, isoalkanes, cycloalkanes, alkenes, aromatics, and PAHs.
- B-5: Selected Specification Properties of Aviation Gas Turbine Fuels. Lists data on composition, volatility, fluidity and combustion for Jet Fuels A and B and JP-4, -5, -7, and -8.
- B-6: Detectable Hydrocarbons Found in U.S. Finished Gasolines at a Concentration of 1% or more. Lists constituents and estimated ranges of weight percentages of each.
- B-7: Major Component Streams of European Automotive Diesel Oil (Diesel Fuel No. 2) and Distillate Marine Diesel Fuel (Diesel Fuel No. 4). Lists nonspecific components by Toxic Substances Control Act (TSCA) inventory name and identification number, as well as volumetric percentages of each in both automotive diesel oil and distillate marine diesel fuel.
- B-8: Henry's Law Constants for Selected Organic Compounds. Lists values of H at 20-25 °C for chlorinated nonaromatics, chlorinated ethers, monocyclic aromatics, pesticides, PCBs, and polycyclic aromatics.

- B-9: Chemical and Physical Properties of TPH Components. Lists molecular weight, water solubility, specific gravity, vapor pressure, Henry's Law constant, diffusivity, Koc, log Kow, Fish Bioconcentration Factor (BCF), and Surface-Water  $T_{1/2}$ , for alcohols, cycloalkanes, cycloalkenes, chlorinated aliphatics, ethers, ketones, methyl alkanes, methyl alkenes, mono- and polycyclic aromatic hydrocarbons, simple alkanes, and simple alkenes.
- B-10: Dimensionless Henry's Law Constants for Typical Organic Compounds. Lists values of H for various compounds at different temperatures.
- B-11: Chemical Properties of Hydrocarbon Constituents. Lists liquid density, Henry's Law Constant, water solubility, vapor pressure, vapor density, and  $K_{oc}$  for n-alkanes, mono-aromatics, phenols, and di-aromatics.
- B-12: Composition of a Regular Gasoline. Lists chemical formula, molecular weight, mass fraction, and mole fraction of 58 components of regular gasoline.
- B-13: Composition of a Weathered Gasoline. Lists same properties as Table B-12 for 58 components of weathered gasoline.

**Table B-1**  
**Selected Compounds and Their Chemical Properties**

Compound	M <sub>w</sub> (g/mole)	T <sub>b</sub> (1 atm) (K)	P <sub>v</sub> ° (K) (atm)	C <sub>est</sub> (mg/l)
n-Pentane	72.2	309	0.57	1700
n-Hexane	86.2	342	0.16	560
Trichloroethane	133.4	348	0.132	720
Benzene	78.1	353	0.10	320
Cyclohexane	84.2	354	0.10	340
Trichloroethylene	131.5	360	0.026	140
n-Heptane	100.2	371	0.046	190
Toluene	92.1	384	0.029	110
Tetrachloroethylene	166	394	0.018	130
n-Octane	114.2	399	0.014	65
Chlorobenzene	113	405	0.012	55
p-Xylene	106.2	411	0.0086	37
Ethylbenzene	106.2	411	0.0092	40
m-Xylene	106.2	412	0.0080	35
o-Xylene	106.2	417	0.0066	29
Styrene	104.1	418	0.0066	28
n-Nonane	128.3	424	0.0042	22.0
n-Propylbenzene	120.2	432	0.0033	16
1,2,4-Trimethylbenzene	120.2	442	0.0019	9.3
n-Decane	142.3	446	0.0013	7.6
Dibromochloropropane	263	469	0.0011	11
n-Undecane	156.3	469	0.0006	3.8
n-Dodecane	170.3	489	0.00015	1.1
Naphthalene	128.2	489	0.00014	0.73
Tetraethyl lead	323	dec. @473K	0.0002	2.6

Note:

M<sub>w</sub> - molecular weight.

T<sub>b</sub>(1 atm) - compound boiling point at 1 atm absolute pressure.

P<sub>v</sub> ° (293 K), - vapor pressure measured at 293 K.

C<sub>est</sub> - equilibrium vapor concentration.

dec. - decomposes

Johnson, Kemblowski, and Colhart (1988). "Practical screening models for soil venting applications." In: *Proceedings of NWWA-API; Conference on Petroleum Hydrocarbons and Organic Chemicals in Groundwater*. Houston, TX. Reprinted by permission of NGWA.

**Table B-2****Physiochemical Properties of PCE and Associated Compounds\***

<b>Formula</b>	<b>PCE <chem>C2Cl4</chem></b>	<b>TCE <chem>C2HCl3</chem></b>	<b>1,1-DCE <chem>C2H2Cl2</chem></b>	<b>t-1,2-DCE <chem>C2H2Cl2</chem></b>	<b>c-1,2-DCE <chem>C2H2Cl2</chem></b>	<b>V C <chem>C2H3Cl</chem></b>
Molecular weight (g/mol)	165.85	131.40	96.95	96.95	96.95	62.5
Liquid density (g/cm <sup>3</sup> )	1.625	1.46	1.214	1.257	1.284	0.9121#
Melting point (K)	250.6	200	150.4	223.6	191.5	119.2
Boiling point (K)	394	360	304.6	320.7	333.2	259.6
Vapor pressure (mmHg)	14	69 <sup>o</sup> 1	500	5.3	2.7	2300
Water solubility (mg/l)	150	1100 <sup>1</sup>	400	6300	3500	1100
Log octanol - water coefficient (K <sub>ow</sub> )	3.14	2.42	2.13	2.09	1.86	1.23
Soil sorption coefficient (K <sub>oc</sub> ) (l/kg)	665	160 <sup>2</sup>	65	59	35	8.2
Henry's Law constant (atm. m <sup>3</sup> /mol)	0.023	.0103 <sup>1</sup>	0.154	0.0066 <sup>1</sup>	0.0075 <sup>1</sup>	0.695

Arthur D. Little, Inc. (1987). *The installation restoration program toxicology guide, Volume 1.* Section 2:1-16.

All values are at 293 K, unless otherwise indicated.

#Value is a specific gravity measurement.

<sup>1</sup>At 298 K.

<sup>2</sup>From Lyman et al.(1982) Handbook of Chemical Property Estimation Methods

**Table B-3**  
**Physiochemical Properties of TCA and Associated Compounds\***

Formula	1,1,1-TCA <chem>C2H3Cl3</chem>	1,1-DCA <chem>C2H4Cl2</chem>	CA <chem>C2H5Cl</chem>
Molecular weight (g/mol)	133.42	98.97	64.52
Liquid density (kg/m <sup>3</sup> )	1.325	1.175	0.921 <sup>1</sup>
Melting point (K)	240	176.3	132.15
Boiling point (K)	347	330.3	285.5
Vapor pressure (mmHg)	100	182	1000
Water solubility (mg/l)	950	5500	5700
Log octanol - water coefficient (K <sub>ow</sub> )	2.49	1.79	1.43
Soil sorption coefficient (K <sub>oc</sub> ) (l/kg)	152	30	14.9
Henry's Law constant (atm. m <sup>3</sup> /mol)	0.0276 <sup>2</sup>	0.0057 <sup>2</sup>	0.011

\*All values are at 293 K, unless otherwise indicated.

<sup>1</sup>At 273 K

<sup>2</sup>At 298 K

Arthur D. Little, Inc. (1987). *The installation restoration program toxicology guide, Volume 1*. Section 2:1-16.

**Table B-4**  
**Physical Properties of Fuel Components**

Component	MW	Solubility	Koc	Log Kow	VP	References
<u>n-Alkanes</u>						
n-Butane	58.12	61			1555.33	///A
n-Decane	142.28	0.009 (20)			2.7	/B//B
n-Dodecane	170.33	0.0037	5500000	7.06	0.3	/A/C/C/A
n-Hexane	86.18	9.5	3830	3.9	121.24	/D/C/C/A
n-Heptane	100.20	2.4 (20)			35.55	/B///A
n-Nonane	128.25	0.07 (20)			3.22	/B//B
n-Octane	114.23	0.0657	73000	4.00	10.46	/E/C/E/A
n-Pentane	72.15	38.5			424.38	/D///A
n-Tridecane	184.35	0.013				/B///
n-Undecane	156.31				1 (32.7)	///B
<u>Isoalkanes</u>						
2-Methyldecane	156.31					///
2-Methylhexane	100.20				51.9	///A
2-Methylpentane	86.18	13.8			171.5	/D///A
2,4-Dimethylhexane	114.23				23.32	///A
2,5-Dimethylhexane	114.23					///
2,2,3-Trimethylpentane	114.23		36000	4.87		//C/C/
2,2,4-Trimethylpentane	114.23	0.56	36000	5.02		/B/C/E/
3-Methylhexane	100.20					///
3-Methylpentane	86.18		3830	3.9		//C/C/
3,4-Dimethyloctane	142.28					///
4-Methylheptane	114.23					///
Isobutane	58.12	48.9			2252.75	/D///A
Isododecane	170.33					///
Isopentane	72.15	47.7	900	2.3	574.89	/E/C/E/A
Isoundecane	156.31					///
<u>Cycloalkanes</u>						
1,3,5-Trimethylcyclohexane	126.24		50500	5.02		//C/C/
Cyclohexane	84.16	55.6	1330	3.44	77.55	/E/C/E/A
Methylcyclohexane	98.19	14 (20)	6070	4.1	144	//C/C/B
Methylcyclopentane	83.15	42.7	1400	2.35		/E/C/E/
<u>Alkenes</u> trans-2-Butene	56.11				760 (0.9)	///B
2-Methyl-2-butene	70.13					///

**Table B-4**  
**(Concluded)**

Component	MW	Solubility	Koc	Log Kow	VP	References
Aromatics	120.19					////
1-Methyl-3-ethylbenzene						
1-Methyl-3-n-propylbenzene	134.22					////
1,2,3-Trimethylbenzene	120.19		2150	4.65		/C/C/
1,2,4-Trimethylbenzene	120.19	57.6	2150	3.65		/E/C/C/
1,3,5-Trimethylbenzene	120.19		2150	3.65	1.73	/C/C/A
1,2,3,4-Tetramethylbenzene	134.22					////
Benzene	78.11	1760	65	2.13	75.2	/E/C/C/A
Ethylbenzene	106.17	152	1200	3.34	7.08	/D/F/F/A
Isopropylbenzene	120.19	50.1		3.43		/E//E/
Toluene	92.14	515	240	2.69	21.84	/E/C/C/A
Xylenes	106.17	175	700	3.16	6/16	/E/C/C/A
PAHs	142.20	27	3570	3.87		B/B/C/C/
1-Methylnaphthalene						
2-Methylnaphthalene	142.20		3570	3.87		B//C/C/
Acenaphthene	154.21	4.09	5250	3.98	0.0016 (25)	B/E/F/F/F
Acenaphthylene	152.20	3.93	2890	3.72	0.03	B/B/F/F/F
Anthracene	178.23	1.29	13500	4.45	0.00024 (25)	B/B/C/E/F
Chrysene	228.20	0.006	220000	5.61	6.3E-09 (25)	B/B/F/F/F
Naphthalene	128.16	31.7	962	3.3	0.09 (25)	B/E/C/C/F
Phenanthrene	178.22	1.24	16000	4.45	9.4E-04 (25)	B/E/F/F/F
Pyrene	202.24	0.15	44000	4.88	2.5E-06 (25)	B/E//E/F

Note:

References

MW/Solubility/Koc/Log Kow/VP

A. EPA, 1989d.

B. Verschueren (1983).

C. IRP (1987).

D. Guard et al. (1983).

E. Lyman, Rechl, and Rosenblatt (1982).

F. A. D. Little (1981).

Solubility in mg/L water at 198 K, unless otherwise noted in parentheses.

Vapor Pressure (VP) of pure compound in mmHg at 20 C, unless otherwise noted in parentheses.

**Table B-5**  
**Selected Specification Properties of Aviation Gas Turbine Fuels<sup>a</sup>**

Characteristic	Civil ASTM D 1655		Military <sup>b</sup>			
			Mil-T-5624-K		Mil-T-38219	Mil-T-83133
	Jet A kerosene	Jet B wide-cut	JP-4 Wide-cut USAF	JP-5 Kerosene USN	JP-7 <sup>c</sup> kerosene USAF	JP-8 Kerosene USAF
Composition						
aromatics, vol. % max	20 <sup>d</sup>	20 <sup>d</sup>	25	25	5	25
sulfur, wt % max	0.3	0.3	0.4	0.4	0.1	0.4
Volatility						
distillation-10% received	204			205	196	205
temperature-50% received		188	190			
max k-endpoint	573		543	563	561	573
vapor pressure at 311 K kPa max (psi)		21(3)	14-21(2-3)			
density at 288 K, kg/m <sup>3</sup>	775-840	751-802	751-802	788-845	779-806	775-840
Fluidity						
freezing-point, k max	233 <sup>e</sup>	223	215	227	230	223
viscosity at 253 K, mm <sup>3</sup> /s max (=cSt)	8.0			8.5	8.0	8.0
Combustion						
heat content, MJ/kg, min	42.8	42.8	42.8	42.6	43.5	42.8
smoke point, mm, min	20 <sup>f</sup>	20 <sup>f</sup>	20	19	35 <sup>c</sup>	20
H <sub>2</sub> content, wt % min			13.6	13.5	14.2 <sup>c</sup>	13.6

Note:

<sup>a</sup>From Dukek (1978); full specification requires other tests.

<sup>b</sup>USAF, US Air Force; USN, US Navy

<sup>c</sup>Estimated properties for advanced supersonic fuel

<sup>d</sup>Fuel up to 25 vol % aromatics may be supplied on notification (22 vol % for Jet A-1, Jet B).

<sup>e</sup>International airlines use Jet A-1 with 223 k freeze-point.

<sup>f</sup>Fuel with 18 smoke point may be supplied on notification (19 for Jet A-1, Jet B).

max = maximum

min = minimum

World Health Organization, International Agency for Research on Cancer. (1989). "IARC monographs on the evaluation of carcinogenic risks to humans – occupational exposures in petroleum refining; crude oil and major petroleum fuels." Volume 45. IARC, Lyon, France.

**Table B-6****Detectable Hydrocarbons Found in U.S. Finished Gasolines at a Concentration of 1% or More<sup>a</sup>**

<b>Chemical</b>	<b>Weight %</b>	
	<b>Estimated Range</b>	<b>Weighted Average<sup>b</sup></b>
Toluene	5-22	10
2-Methylpentane		
+ 4-Methyl-cis-2-pentene	4-14	9
+ 3-Methyl-cis-2-pentene <sup>c</sup>		
n-Butane	3-12	7
iso-Pentane	5-10	7
n-Pentane	1-9	5
Xylene (three isomers)	1-10	3
2,2,4-Trimethylpentane	<1-8	3
n-Hexane	<1-6	2
n-Heptane	<1-5	2
2,3,3-Trimethylpentane	<1-5	2
2,3,4-Trimethylpentane	<1-5	2
3-Methylpentane	<1-5	2
Methylcyclohexane		
+ 1-cis-2-Dimethylcyclopentane	<1-5	1
+ 3-Methylhexane <sup>c</sup>		
Benzene	<1-4	2
2,2,3-Trimethylpentane	<1-4	2
Methyl tertiary butyl ether (MTBE)	<1-4	1
Methylcyclopentane	<1-3	2
2,4-Dimethylpentane	<1-3	1
Cyclohexane	<1-3	1
1,2,4-Trimethylbenzene	<1-3	1
2-Methyl-2-butene	<1-2	2
2,3-Dimethylbutane	<1-2	1
Trans-2-Pentene	<1-2	1
Methylcyclohexane	<1-2	1
3-Ethyltoluene	<1-2	1
2,3-Dimethylpentane	<1-2	1
2,5-Dimethylpentane	<1-2	1
2-Methyl-1-butene	<1-2	1
Ethyl benzene	<1-2	1

<sup>a</sup>Provided by American Petroleum Institute<sup>b</sup>The sum of the weighted average does not equal 100% because numerous components were detected at less than 1%.<sup>c</sup>These chemicals could not be distinguished by gas chromatography because of similar retention times.

**Table B-7**

**Major Component Streams of European Automotive Diesel Oil (Diesel Fuel No. 2) and Distillate Marine Diesel Fuel (Diesel Fuel No. 4)<sup>a</sup>**

Toxic Substances Control Act (TSCA) Inventory Name and Identification Number <sup>b</sup>	Refinery Process Stream (nomenclature used in Europe)	Automotive Diesel Oil (vol. %)	Distillate Marine Diesel Fuel (vol. %)
Straight-run middle distillate [6]	Straight-run (atmospheric) gas oil	40-100	40-100
Straight-run gas oil [7]	- light - heavy	0-3	0-50
Light vacuum distillate [19]	Vacuum gas oil	0-10	0-20
Light thermally cracked distillate [30]	Thermally cracked gas oil	0-20	0-30
Light catalytically cracked distillate [24]	Light catalytically cracked gas oil (cycle oil)	0-25	0-40

<sup>a</sup>From CONCAWE (1985).

<sup>b</sup>The numbers in brackets correlate with these products in Figure 1 and Table 2 in the monograph Occupational Exposures in Petroleum Refining, contained in the reference cited below.

World Health Organization, International Agency for Research on Cancer. (1989). "ARC monographs on the evaluation of carcinogenic risks to humans - occupational exposures in petroleum refining; crude oil and major petroleum fuels." Volume 45. IARC, Lyon, France.

**Table B-8**

Henry's Law Constants ( $H$ , atm-m<sup>3</sup>/mol) for Selected Organic Compounds [Data Obtained from Mabey et al. (1982) and Mackay and Shiu (1981)]

Compound	$H$	$t$ (K) <sup>a</sup>	Compound	$H$	$t$ (K) <sup>a</sup>
<b>Chlorinated Nonaromatics</b>					
Benzene	0.0055	298	Naphthalene	0.00046	298
Chlorobenzene	0.0036	293/298	Acenaphthene	0.000091	298
o-Dichlorobenzene	0.0019	293	Acenaphthylene	0.0015	293/298
m-Dichlorobenzene	0.0036	298	Anthracene	0.000086	298
p-Dichlorobenzene	0.0031	298	Phenanthrene	0.00023	298
1,2,4-Trichlorobenzene	0.0023	298			
Methyl chloride	0.04	293	Hexachlorobenzene	0.00068	293/298
Methyl bromide	0.20	293	Toluene	0.0067	293
Methylene chloride	0.0020	293/298	Ethylbenzene	0.0066	293
Chloroform	0.0029	293	o-Xylene	0.0050	298
Bromodichloromethane	0.0024	293/295	m-Xylene	0.0070	298
Dibromochloromethane	0.00099	293/295	p-Xylene	0.0071	298
Bromoform	0.00056	293	1,2,3-Trimethylbenzene	0.0032	298
Dichlorodifluoromethane	3.0	298	1,2,4-Trimethylbenzene	0.0059	298
Trichlorofluoromethane	0.11	293	1,3,5-Trimethylbenzene	0.0060	298
Carbon tetrachloride	0.023	293	Propylbenzene	0.0070	298
Chloroethane	0.15	293	Isopropylbenzene	0.0013	298
1,1-Dichloroethane	0.0043	293	1-Ethyl-2-methylbenzene	0.0043	298
1,2-Dichloroethane	0.00091	293	1-Ethyl-4-methylbenzene	0.0050	298
1,1,1-Trichloroethane	0.03	298	n-Butylbenzene	0.013	298
1,1,2-Trichloroethane	0.00074	293	Isobutylbenzene	0.033	298
1,1,2,2-Tetrachloroethane	0.00038	293	sec-Butylbenzene	0.014	298
Hexachloroethane	0.0025	293/295	tert-Butylbenzene	0.012	298
Vinyl chloride	0.081	298	1,2,4,5-Tetramethylbenzene	0.025	298
1,1-Dichloroethene	0.19	298/293	1-Isopropyl-4-methylbenzene	0.0080	298
1,2-trans-Dichloroethene	0.067	293	n-Pentylbenzene	0.0060	298
Trichloroethene	0.0091	293	<b>Pesticide and Related Compounds, and PCBs</b>		
Tetrachloroethene	0.0153	293	Ethylene dibromide (EDB) <sup>b</sup>	0.00082	298
1,2-Dichloropropane	0.0023	293	trans-Chlordane	0.000094	298

**Table B-8**  
**(Concluded)**

trans-1,3-Dichloropropene	0.0013	293/298	Heptachlor	0.0040	298
Hexachlorocyclopentadiene	0.016	298	Heptachlor epoxide	0.00039	298
Hexachlorobutadiene	0.026	293	2,3,7,8-TCDD	0.0021	--
<b>Chlorinated Ethers</b>			Aroclor 1016 <sup>c</sup>	0.00033	298
Bis(chloromethyl)ether	0.00021	293/298	Aroclor 1221 <sup>c</sup>	0.00017	298
Bis(2-chloroisopropyl)ether	0.00011	293	Aroclor 1242 <sup>c</sup>	0.0020	298
4-Chlorophenylphenylether	0.00022	293	Aroclor 1248 <sup>c</sup>	0.0036	298
4-Bromophenylphenylether	0.00010	293/298	Aroclor 1254 <sup>c</sup>	0.0026	--

<sup>a</sup>Where two temperatures are given, the first is the temperature at which the vapor pressure was measured, and the second is the temperature at which the solubility was measured.

<sup>b</sup>Vapor pressure data from Stull (1947), and solubility data from Stephen and Stephen (1963).

<sup>c</sup>Mixture-average value.

Pankow, J. F., Johnson, R. L., and Cherry, J. A. (1993). Air sparging in gate wells in cutoff walls and trenches for control of volatile organics, *Ground Water* 31(4):654-63. Reprinted by permission of Ground Water Publishing Company.

**Table B-9**  
**Chemical and Physical Properties of TPH Components**

Constituents	Molecular Weight	Water Solubility mg/L 298 K	Specific Gravity	Vapor Pressure mm Hg 298 K	Henry's Law Constant atm-m <sup>3</sup> /mol 298 K	Diffusivity cm <sup>2</sup> /sec	K <sub>oc</sub> mL/g	Log K <sub>ow</sub>	Fish BCF L/kg	Surface-Water T <sub>1/2</sub> (days)
										Low -High
<b>Alcohols</b>										
Ethyl alcohol	46.07	280,000	0.789	59	1.2E-05	0.12368	0.3	3.1	0.34	
Methyl alcohol	32	300,000		130	2.0E-05	0.16211	0.1	1.5	2.3	
t-Butyl alcohol	74.1		0.788	42		0.09752		0.37		
<b>Cycloalkanes</b>										
Cyclopentane	70.14	160	0.751	42.4	1.9E+01					
Methyl cyclohexane	98.19	14	0.77	6.18	4.3E+01					
<b>Cycloalkenes</b>										
Cyclohexene	84.16	55 (20°C)	0.779							
Cyclopentene	68.12		0.77	77 (20°C)						
<b>Chlorinated Aliphatics</b>										
1,2-Dichloroethane	99	7,986-8,650	1.23	87	1.3E-03	0.09451	65	1.48-2.13	5.6	28-180
Dibromoethane	187.88	4.32 (30°C)	2.701	17 (30°C)						
1,1-Dichloroethane	99	5,060	1.1757	182.1	5.9E-03	0.0959	30.2	1.79		
<b>Ether</b>										
Methyl-t-butyl ether (MTBE)	88	4,800	0.74	250	5.9E-03	0.10172	41	1.2	1.5	28-180
<b>Ketones</b>										
Methyl isobutyl ketone	100.2	20,400	0.8017	14.5	9.4E-05	0.07588	19 to 106	1.19		
<b>Methyl Alkanes</b>										
2,3-Dimethylbutane	86.7	19.1		31.3	1.3E+02					
2,3-Dimethylpentane	100.21	5.25		9.18	1.8E+02					

Table B-9

(Continued)

Constituents	Molecular Weight	Water Solubility mg/L 298 K	Specific Gravity	Vapor Pressure mm Hg 298 K	Henry's Law Constant atm-m <sup>3</sup> /mol 298 K	Diffusivity cm <sup>2</sup> /sec	K <sub>oc</sub> mL/g	Log K <sub>ow</sub>	Fish BCF L/kg	Surface-Water T <sub>1/2</sub> (days)
										Low -High
2,4-Dimethylpentane	100.21	5.5		13.1	3.0E+02					
3,3-Dimethylpentane	100.21	5.94		11	1.9E+02					
2-Methylheptane	114.23									
3-Methylheptane	114.23	0.792		2.6	3.8E+02					
4-Methylheptane	114.23									
2-Methylhexane	100.21	2.54		8.78	3.5E+02					
3-Methylhexane	100.21	4.95		8.21	2.4E+02					
4-Methyloctane	128.26	0.115		0.903	1.0E+03					
2-Methylpentane	86.17	13	0.654	28.2	1.7E+02					
3-Methylpentane	86.17	13.1	0.6645	25.3	1.7E+02					
2,2,4-Trimethylhexane	128.26									
2,2,5-Trimethylhexane	128.26	1.15		2.21	3.5E+02					
2,3,3-Trimethylhexane	128.26									
2,3,5-Trimethylhexane	128.26									
2,4,4-Trimethylhexane	128.26									
2,2,3-Trimethylpentane	114.23									
2,2,4-Trimethylpentane	114.23	2.44		6.56	3.3E+02					
2,3,3-Trimethylpentane	114.23									
2,3,4-Trimethylpentane	114.23	2.3		3.6	1.9E+02					
<b>Methyl Alkenes</b>										
2-Methyl-1-butene		70.14		0.65						
2-Methyl-2-butene	70.14		0.668							

**Table B-9**  
**(Continued)**

Constituents	Molecular Weight	Water Solubility mg/L 298 K	Specific Gravity	Vapor Pressure mm Hg 298 K	Henry's Law Constant atm-m <sup>3</sup> /mol 298 K	Diffusivity cm <sup>2</sup> /sec	K <sub>oc</sub> mL/g	Log K <sub>ow</sub>	Fish BCF L/kg	Surface-Water T <sub>1/2</sub> (days)
										Low -High
3-Methyl-1-butene	70.14	130	0.648	120	5.5E+01					
2-Methyl-1-pentene	86.16	78	0.6817							
2-Methyl-2-pentene	86.16									
3-Methyl-cis-2-pentene	86.16									
3-Methyl-trans-2-pentene	86.16			0.67						
4-Methyl-cis-2-pentene	86.16			0.67						
4-Methyl-trans-2-pentene	86.16									
<b>Monocyclic Aromatic Hydrocarbons</b>										
Benzene	78	1.780	0.88	95	5.5E-03	9.30E-02	49 to 100	1.56 to 2.15	5.2	5
Butylbenzene	134		0.86	1 (23°C)			1,500			
n-Butylbenzene	134	50	0.86	1 (23°C)	1.3E+00					
sec-Butylbenzene	134	30.9	0.87	1.5 (20°C)	1.4E+00					
t-Butylbenzene	134	34	0.862	1.1 (20°C)	1.2E+00					
1,2-Diethylbenzene	136						1,500			
1,3-Diethylbenzene	136						1,500			
Ethylbenzene	106	152 to 208	0.87	9.5	8.7E-03	6.70E-02	95 to 260	3.05 to 3.15	37.5	3
Isobutylbenzene	134.2	10.1		0.248	3.3E+00					
eip-Isopropylbenzene	120	50 (20°C)	0.862	3.2 (20°C)	1.0E-02			3.66		2
n-Pentylbenzene	149						2,520			
Propylbenzene	120.2	60		0.449	7.0E-1					
n-Propylbenzene	120	60 (15C)	0.862	2.5 (20°C)	5.6E-03 (15°C)			3.57 to 3.68		
1,2,3,4-Tetramethylbenzene	215.9	4.31		0.00876	2.6E-01		1,500			

**Table B-9**  
(Continued)

Constituents	Molecular Weight	Water Solubility mg/L 298 K	Specific Gravity	Vapor Pressure mm Hg 298 K	Henry's Law Constant atm-m <sup>3</sup> /mol 298 K	Diffusivity cm <sup>2</sup> /sec	K <sub>oc</sub> mL/g	Log K <sub>ow</sub>	Fish BCF L/kg	Surface-Water T <sub>1/2</sub> (days)
										Low -High
<b>Polycyclic Aromatic Hydrocarbons</b>										
Anthracene	178	0.030 to 0.1125	1.24	1.7E-05 to 1.95E-4	6.5E-05	5.90E-02	16,000 to 26,000	4.34 to 4.54	30	0.071/0.024
Benzo(a)pyrene	252	0.0038 to 0.004	1.35	5.5E-09	<2.4E-6	4.70E-02	398,000 to 1,900,000	5.81 to 6.50	30	0.015/0.046
Benzo(b)fluoranthene	252	0.0012	ND	5.0E-07	1.2E-05	4.40E-02	550,000	6.57	ND	0.36
Benzo(e)pyrene	252					4.70E-02				
1,2-Dimethylnaphthalene	158						4,230			
1,3-Dimethylnaphthalene	158						4,230			
Fluoranthene	202	0.206 to 0.373	1.25	0.000005	1.7E-02	4.2E-02	5.22	1,150	0.875	2.6
Fluorene	166	1.66 to 1.98	1.2	1E-3 to 1E-2	2.1E-04	5.70E-02	5,000	4.12 to 4.38	30	32
Methylnaphthalene	142	27								
1-Methylnaphthalene	142	28	1.025	ND	ND	ND	ND	ND	129	ND
2-Methylnaphthalene	142	25	1.001	0.045	3.4E-04	6.20E-02	7,400 to 8,500	3.86 to 4.11	190	ND
Naphthalene	128	30 to 34	1.16	2.3E-1 to 8.7E-1	4.6E-04	8.20E-02	550 to 3,160	3.2 to 4.7	10.5	0.5
Phenanthrene	178	0.71 to 1.29	1.18	0.00068	2.6E-05	5.40E-02	5,250 to 38,900	4.2 to 4.6	30	0.125/1.04
Pyrene	202	0.013 to 0.171	1.27	6.85E-07 to 2.5E-06	1.1E-05	5.00E-02	46,000 to 135,000	4.88 to 5.32	30	0.028/0.085
<b>Simple Alkanes</b>										
n-Butane	58.13	61	0.6	1.82E+03	9.6E-01					
Decane	148.28	0.008								
n-Decane	148.28	0.052		1.31	7.0E+00					
Dodecane	170.33	0.0037		0.0118	7.5E+00					
n-Dodecane	170.33									
n-Eicosane	282.6	0.0019		2.67E-06	2.9E-01					

**Table B-9**  
**(Continued)**

Constituents	Molecular Weight	Water Solubility mg/L 298 K	Specific Gravity	Vapor Pressure mm Hg 298 K	Henry's Law Constant atm-m <sup>3</sup> /mol 298 K	Diffusivity cm <sup>2</sup> /sec	K <sub>OC</sub> mL/g	Log K <sub>OW</sub>	Fish BCF L/kg	Surface-Water T <sub>1/2</sub> (days)
										Low -High
n-Heptane	100.21	3		0.515	2.3E+00					
n-Hexadecane	226.44	0.00628		0.00917	2.3E+01					
n-Hexane	86	18 (20°C)	0.66	1.2E-2 (20°C)	7.7E-01	7.50E-02	890	2.77	ND	ND
Isobutane	58.13	48.19		2,678	1.2E+00					
Isopentane	72.15	48		695	1.4E+00					
n-Nonane	128.26	0.07		4.281	5.0E+00					
n-Octadecane	254.4	0.0021		2.50E-05	2.9E+00					
n-Octane	114.23	0.66		14	3.0E+00					
n-Pentane	72.15	35		513	1.3E+00					
Propane	44.09	63	0.58	64						
n-Tetradecane	190.38	0.00696		0.0095	1.1E+00					
Undecane	156.32	0.044		0.39	1.9E+01					
n-Undecane	156.32									
Simple Alkenes										
2-Butene		210								
cis-2-Butene	56.1		0.6							
trans-2-Butene	56.1		0.64							
cis-3-Heptene	98	9								
trans-3-Heptene	98									
cis-2-Hexene	84	50	0.86							
trans-2-Hexene	84	50	0.86							
cis-3-Hexene	84									
trans-3-Hexene	84									

**Table B-9**  
**(Continued)**

<b>Constituents</b>	<b>Molecular Weight</b>	<b>Water Solubility mg/L 298 K</b>	<b>Specific Gravity</b>	<b>Vapor Pressure mm Hg 298 K</b>	<b>Henry's Law Constant atm-m<sup>3</sup>/mol 298 K</b>	<b>Diffusivity cm<sup>2</sup>/sec</b>	<b>K<sub>oc</sub> mL/g</b>	<b>Log K<sub>ow</sub></b>	<b>Fish BCF L/kg</b>	<b>Surface-Water T<sub>1/2</sub> (days)</b>
										<b>Low -High</b>
1-Pentene	70.14	150		85	4.0E+01					
2-Pentene	70.14	203		66	2.3E+01					
cis-2-Pentene	70.14									
trans-2-Pentene	70.14									

Note:

BCF - Bioconcentration factor

T<sub>1/2</sub> - half life

Heath, J. S., Koblis, K., Sager, S. L., and Day, C. (1993). Risk assessment for total petroleum hydrocarbons. Calabrese, E. J., and Kostecki, P. T. (eds.). *Hydrocarbon Contaminated Soils - Volume III*. Lewis Publishers, Chelsea, MI. pp. 267-301. Reprinted by permission of Lewis Publishers, an imprint of CRC Press, Boca Raton, FL.

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**Table B-10**  
**Dimensionless Henry's Law Constants for Typical Organic Compounds**

Component	283 K	289 K	293 K	298 K	303 K
Nonane	17.21519	20.97643	13.80119	16.92131	18.69235
n-Hexane	10.24304	17.46626	36.70619	31.39026	62.70981
2-Methylpentane	29.99747	29.35008	26.31372	33.72000	34.08841
Cyclohexane	4.43291	5.32869	5.81978	7.23447	8.96429
Chlorobenzene	0.10501	0.11884	0.14175	0.14714	0.19014
1,2-Dichlorobenzene	0.07015	0.06048	0.06984	0.06417	0.09527
1,3-Dichlorobenzene	0.09511	0.09769	0.12222	0.11649	0.16964
1,4-Dichlorobenzene	0.09124	0.09177	0.10767	0.12957	0.15637
o-Xylene	0.12266	0.15267	0.19704	0.19905	0.25164
p-Xylene	0.18076	0.20427	0.26813	0.30409	0.37988
m-Xylene	0.17689	0.20976	0.24859	0.30409	0.35656
Propylbenzene	0.24446	0.30915	0.36623	0.44143	0.55072
Ethylbenzene	0.14030	0.19073	0.24983	0.32208	0.42209
Toluene	0.16397	0.20807	0.23071	0.26240	0.32480
Benzene	0.14203	0.16409	0.18790	0.21581	0.28943
Methylethylbenzene	0.15106	0.17762	0.20910	0.22807	0.30953
1,1-Dichloroethane	0.15838	0.19200	0.23404	0.25545	0.31194
1,2-Dichloroethane	0.05035	0.05498	0.06111	0.05763	0.06995
1,1,1-Trichloroethane	0.41532	0.48635	0.60692	0.71119	0.84819
1,1,2-Trichloroethane	0.01678	0.02664	0.03076	0.03719	0.05346
cis-1,2-Dichloroethylene	0.11620	0.13787	0.14965	0.18556	0.23114
trans-1,2-Dichloroethylene	0.25390	0.29815	0.35625	0.38625	0.48640
Tetrachloroethylene	0.36410	0.46943	0.58614	0.69892	0.98487
Trichloroethylene	0.23154	0.28208	0.35002	0.41690	0.51454
Tetralin	0.03228	0.04441	0.05654	0.07643	0.10773
Decalin	3.01266	3.53977	4.40641	4.78211	7.99952
Vinyl chloride	0.64557	0.71049	0.90207	1.08313	1.12556
Chloroethane	0.32666	0.40515	0.45727	0.49456	0.57484
Hexachloroethane	0.25522	0.23641	0.24568	0.34129	0.41405
Carbon tetrachloride	0.63696	0.80776	0.96442	1.20575	1.51951
1,3,5-Trimethylbenzene	0.17344	0.19454	0.23736	0.27507	0.38711

**Table B-10**  
**(Concluded)**

Component	283 K	289 K	293 K	298 K	303 K
Ethylene dibromide	0.01291	0.02030	0.02536	0.02657	0.03216
1,1-Dichloroethylene	0.66278	0.85851	0.90622	1.05860	1.27832
Methylene chloride	0.06025	0.07147	0.10143	0.12098	0.14512
Chloroform	0.07403	0.09854	0.13801	0.17207	0.22270
1,1,2,2-Tetrachloroethane	0.01420	0.00846	0.03035	0.01022	0.02814
1,2-Dichloropropane	0.05251	0.05329	0.07898	0.14592	0.11497
Dibromochloromethane	0.01635	0.01903	0.04282	0.04823	0.06110
1,2,4-Trichlorobenzene	0.05552	0.04441	0.07607	0.07848	0.11939
2,4-Dimethylphenol	0.35678	0.28504	0.41986	0.20150	0.15074
1,1,2-Trichlorotrifluoroethane	6.62785	9.09260	10.18462	13.03840	12.90375
Methyl ethyl ketone	0.01205	0.01649	0.00790	0.00531	0.00442
Methyl isobutyl ketone	0.02841	0.01565	0.01206	0.01594	0.02734
Methyl cellosolve	1.89798	1.53517	4.82210	1.26297	1.53277
Trichlorofluoromethane	2.30684	2.87580	3.34222	4.12815	4.90423

Source: USEPA (1991d). (Adapted from Howe, Mullins, and Rogers (1986)).

**Table B-11**  
**Chemical Properties of Hydrocarbon Constituents**

Chemical Class	Representative Chemical	Liquid Density (g/cm <sup>3</sup> ) @ 293 K	Henry's Law Constant (dim.)	Water Solubility (mg/l) @ 293 K	Pure Component Vapor Pressure (mm Hg) 293 K	Vapor Density (g/m <sup>3</sup> ) @ 293 K	Soil Sorption Constant (K <sub>oc</sub> ) (L/kg) @ 298 K
<b>n-Alkanes</b>							
C4		0.579	25.22	61.1	1560	4960	250
C5	n-Pentane	0.626	29.77	41.2	424	1670	320
C6	n-Hexane	0.659	36.61	12.5	121	570	600
C7	n-Heptane	0.684	44.60	2.68	35.6	195	1300
C8	n-Octane	0.703	52.00	0.66	10.5	65.6	2600
C9	n-Nonane	0.718	NA	0.122	3.2	22.4	5800
C10	n-Decane	0.730	NA	0.022	0.95	7.4	13000
<b>Mono-aromatics</b>							
C6		0.885	0.11	1780	75.2	321	38
C7	n-Butane	0.867	0.13	515	21.8	110	90
C8	m-Xylene	0.864	0.12	162	6.16	35.8	220
C8	Ethylbenzene	0.867	0.14	167	7.08	41.1	210
C9	1,3,5-Trimethylbenzene	0.865	0.09	72.6	1.73	11.4	390
C10	1,4-Diethylbenzene	0.862	0.19	15	0.697	5.12	1100
<b>Phenols</b>							
Phenol	Phenol	1.058	0.038	82000	0.529	2.72	110
C1-Phenols	m-Cresol	1.027	0.044	23500	0.15	0.89	8.4
C2-Phenols	2,4-Dimethylphenol	0.965	0.048	1600	0.058	0.39	NA
C3-Phenols	2,4,6-Trimethylphenol	NA	NA	NA	0.012	0.09	NA
C4-Phenols	m-Ethylphenol	1.037	NA	NA	0.08	0.53	NA
Indanol	Indanol	NA	NA	NA	0.014	0.1	NA
Di-aromatics	Naphthalene	1.025	NA	30	0.053	0.37	690

Note:NA - Not available

dim. - dimensionless

Source: USEPA (1991d).

**Table B-12**  
**Composition of a Regular Gasoline**

<b>Component Number</b>	<b>Chemical Formula</b>	<b>MW (g)</b>	<b>Initial</b>	
			<b>Mass Fraction</b>	<b>Mole Fraction</b>
Propane	C3H8	44.1	0.0001	0.0002
Isobutane	C4H10	58.1	0.0122	0.1999
n-Butane	C4H10	58.1	0.0629	0.1031
trans-2-Butene	C4H10	56.1	0.0007	0.0012
cis-2-Butene	C4H10	56.1	0.0000	0.0000
3-Methyl-1-butene	C5H10	70.1	0.0006	0.0008
Isopentane	C5H12	72.2	0.1049	0.1384
1-Pentene	C5H10	70.1	0.0000	0.0000
2-Methyl-1-butene	C5H10	70.1	0.0000	0.0000
2-Methyl-1,3-butadiene	C5H8	68.1	0.0000	0.0000
n-Pentane	C5H12	72.2	0.0586	0.0773
trans-2-Pentene	C5H10	70.1	0.0000	0.0000
2-Methyl-2-butene	C5H10	70.1	0.0044	0.0060
3-Methyl-1,2-butadiene	C5H8	68.1	0.0000	0.0000
3,3-Dimethyl-1-butene	C6H12	84.2	0.0049	0.0055
Cyclopentane	C5H10	70.1	0.0000	0.0000
3-Methyl-1-pentene	C6H12	84.2	0.0000	0.0000
2,3-Dimethylbutane	C6H14	86.2	0.0730	0.0807
2-Methylpentane	C6H14	86.2	0.0273	0.0302
3-Methylpentane	C6H14	86.2	0.0000	0.0000
n-Hexane	C6H14	86.2	0.0283	0.0313
Methylcyclopentane	C6H12	84.2	0.0000	0.0000
2,2-Dimethylpentane	C7H16	100.2	0.0076	0.0093
Benzene	C6H6	78.1	0.0076	0.0093
Cyclohexane	C6H12	84.2	0.0000	0.0000
2,3-Dimethylpentane	C7H16	100.2	0.0390	0.0371
3-Methylhexane	C7H16	100.2	0.0000	0.0000
3-Ethylpentane	C7H16	100.2	0.0000	0.0000
2,2,4-Trimethylpentane	C8H18	114.2	0.0121	0.0101
n-Heptane	C7H16	100.2	0.0063	0.0060
Methylcyclohexane	C7H14	98.2	0.0000	0.0000

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**Table B-12**  
**(Concluded)**

Component Number	Chemical Formula	MW (g)	Initial	
			Mass Fraction	Mole Fraction
2,2-Dimethylhexane	C8H18	114.2	0.0055	0.0046
Toluene	C7H8	92.1	0.0550	0.0568
2,3,4-Trimethylpentane	C8H18	114.2	0.0121	0.0101
2-Methylheptane	C8H18	114.2	0.0155	0.0129
3-Methylheptane	C8H18	114.2	0.0000	0.0000
n-Octane	C8H18	114.2	0.0013	0.0011
2,4,4-Trimethylhexane	C9H20	128.3	0.0087	0.0065
2,2-Dimethylheptane	C9H20	128.3	0.0000	0.0000
p-Xylene	C8H10	106.2	0.0957	0.0858
m-Xylene	C8H10	106.2	0.0000	0.0000
3,3,4-Trimethylhexane	C9H20	128.3	0.0281	0.0209
o-Xylene	C8H10	106.2	0.0000	0.0000
2,2,4-Trimethylheptane	C10H22	142.3	0.0105	0.0070
3,3,5-Trimethylheptane	C10H22	142.3	0.0000	0.0000
n-Propylbenzene	C9H12	120.2	0.0841	0.0666
2,3,4-Trimethylheptane	C10H22	142.3	0.0000	0.0000
1,3,5-Trimethylbenzene	C9H12	120.2	0.0411	0.0325
1,2,4-Trimethylbenzene	C9H12	120.2	0.0213	0.0169
Methylpropylbenzene	C10H14	134.2	0.0351	0.0249
Dimethylethylbenzene	C10H14	134.2	0.0307	0.0218
1,2,4,5-Tetramethylbenzene	C10H14	134.2	0.0133	0.0094
1,2,3,4-Tetramethylbenzene	C10H14	134.2	0.0129	0.0091
1,2,4-Trimethyl-5-ethylbenzene	C11H16	148.2	0.0405	0.0260
n-Dodecane	C12H26	170.3	0.0230	0.0129
Naphthalene	C10H8	128.2	0.0045	0.0033
n-Hexylbenzene	C12H20	162.3	0.0000	0.0000
Methylnaphthalene	C11H10	142.2	0.0023	0.0015
Total			0.9917	1.0000

Johnson, P. C., Kembrowski, M. W., and Colthart, J. D. (1990b). "Quantitative analysis for the cleanup of hydrocarbon-contaminated soils by in-situ venting," *Ground Water* 28(3):413-29. Reprinted by permission of Ground Water Publishing Company.

**Table B-13**  
**Composition of a Weathered Gasoline**

<b>Component Number</b>	<b>Chemical Formula</b>	<b>MW (g)</b>	<b>Initial</b>	
			<b>Mass Fraction</b>	<b>Mole Fraction</b>
Propane	C3H8	44.1	0.0000	0.0000
Isobutane	C4H10	58.1	0.0000	0.0000
n-Butane	C4H10	58.1	0.0000	0.0000
Trans-2-Butene	C4H10	56.1	0.0000	0.0000
cis-2-Butene	C4H10	56.1	0.0000	0.0000
3-Methyl-1-butene	C5H10	70.1	0.0000	0.0000
Isopentane	C5H12	72.2	0.0200	0.0290
1-Pentene	C5H10	70.1	0.0000	0.0000
2-Methyl-1-butene	C5H10	70.1	0.0000	0.0000
2-Methyl-1,3-butadiene	C5H8	68.1	0.0000	0.0000
n-Pentane	C5H12	72.2	0.0114	0.0169
trans-2-Pentene	C5H10	70.1	0.0000	0.0000
2-Methyl-2-butene	C5H10	70.1	0.0000	0.0000
3-Methyl-1,2-butadiene	C5H8	68.1	0.0000	0.0000
3,3-Dimethyl-1-butene	C6H12	84.2	0.0000	0.0000
Cyclopentane	C5H10	70.1	0.0000	0.0000
3-Methyl-1-pentene	C6H12	84.2	0.0000	0.0000
2,3-Dimethylbutane	C6H14	86.2	0.0600	0.0744
2-Methylpentane	C6H14	86.2	0.0000	0.0000
3-Methylpentane	C6H14	86.2	0.0000	0.0000
n-Hexane	C6H14	86.2	0.0370	0.0459
Methylcyclopentane	C6H12	84.2	0.0000	0.0000
2,2-Dimethylpentane	C7H16	100.2	0.0000	0.0000
Benzene	C6H6	78.1	0.0100	0.0137
Cyclohexane	C6H12	84.2	0.0000	0.0000
2,3-Dimethylpentane	C7H16	100.2	0.1020	0.1088
3-Methylhexane	C7H16	100.2	0.0000	0.0000
3-Ethylpentane	C7H16	100.2	0.0000	0.0000
2,2,4-Trimethylpentane	C8H18	114.2	0.0000	0.0000
n-Heptane	C7H16	100.2	0.0800	0.0853
Methylcyclohexane	C7H14	98.2	0.0000	0.0000

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**Table B-13**  
**(Concluded)**

Component Number	Chemical Formula	MW (g)	Initial	
			Mass Fraction	Mole Fraction
2,2-Dimethylhexane	C8H18	114.2	0.0000	0.0000
Toluene	C7H8	92.1	0.1048	0.1216
2,3,4-Trimethylpentane	C8H18	114.2	0.0000	0.0000
2-Methylheptane	C8H18	114.2	0.0500	0.0468
3-Methylheptane	C8H18	114.2	0.0000	0.0000
n-Octane	C8H18	114.2	0.0500	0.0468
2,4,4-Trimethylhexane	C9H20	128.3	0.0000	0.0000
2,2-Dimethylheptane	C9H20	128.3	0.0000	0.0000
p-Xylene	C8H10	106.2	0.1239	0.1247
m-Xylene	C8H10	106.2	0.0000	0.0000
3,3,4-Trimethylhexane	C9H20	128.3	0.0250	0.0208
o-Xylene	C8H10	106.2	0.0000	0.0000
2,2,4-Trimethylheptane	C10H22	142.3	0.0000	0.0000
3,3,5-Trimethylheptane	C10H22	142.3	0.0250	0.0188
n-Propylbenzene	C9H12	120.2	0.0829	0.0737
2,3,4-Trimethylheptane	C10H22	142.3	0.0000	0.0000
1,3,5-Trimethylbenzene	C9H12	120.2	0.0250	0.0222
1,2,4-Trimethylbenzene	C9H12	120.2	0.0250	0.0222
Methylpropylbenzene	C10H14	134.2	0.0373	0.0297
Dimethylethylbenzene	C10H14	134.2	0.0400	0.0319
1,2,4,5-Tetramethylbenzene	C10H14	134.2	0.0400	0.0319
1,2,3,4-Tetramethylbenzene	C10H14	134.2	0.0000	0.0000
1,2,4-Trimethyl-5-ethylbenzene	C11H16	148.2	0.0000	0.0000
n-Dodecane	C12H26	170.3	0.0288	0.0181
Naphthalene	C10H8	128.2	0.0100	0.0083
n-Hexylbenzene	C12H20	162.3	0.0119	0.0078
Methylnaphthalene	C11H10	142.2	0.0000	0.0000
Total			1.0000	1.0000

Johnson, P. C., Kembowski, M. W., and Colhart, J. D. (1990b). "Quantitative analysis for the cleanup of hydrocarbon-contaminated soils by in-situ venting," *Ground Water* 28(3):413-29. Reprinted by permission of Ground Water Publishing Company.